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On elastic morse scattering

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Some calculations have been presented here on elastic scattering by Morse potentia by some well-known methods. The influence of Coulomb field on Morse scattering has been discussed in the first approximation and the Schrodinger equation for S-wave scattering also solved rigorously.

1. Introduction

We propose to present here some calculations on elastic scattering by Morse potential by some well-known methods. In order to explain the spectra produced by diatomic molecules, Morse (1929) introduced the atomic potential

$$V(r)=V_0\{1-e^{-\alpha(r-r_0)}\}^2 \qquad \ldots(1)$$

We shall not, however, adopt this form in our discussions. The following equivalent form (Landau & Lifshitz, 1958) will be used,

$$V(r)=V_0\{e^{-2\alpha(r-r_0)}-2e^{-\alpha(r-r_0)}\} \qquad \ldots(2)$$

Here r_0 is the distance where the potential is minimum, $-V_0$. α gives a measure of the range of the potential. Evidently, Morse potential is a short-range potential.

2. Scattering Amplitude

In the first Born approximation, the scattering amplitude is given (Kursunoglu 1962, Mott & Massey 1949) by,

$$f(\theta)=-\frac{2m}{K\hbar^2}\int_0^\infty r.\ \sin Kr.\ V_0\left(e^{-2\alpha(r-r_0)}-2\,e^{-\alpha(r-r_0)}\right)$$

$$=-\frac{8mV_0\alpha}{\hbar^2}\left[\frac{e^{2\alpha r_0}}{(K^2+4\alpha^2)^2}-\frac{e^{\alpha r_0}}{(K^2+\alpha^2)^2}\right] \qquad \ldots(3)$$

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where m is the reduced mass and $K = 2\,k \sin \theta/2$, k being the momentum and θ the angle of scattering.

Now we consider two extreme cases (subject to the validity discussed in the next section) :

(a) For $K/\alpha \gg 1$

$$f(\theta) = -\frac{8mV_0\alpha}{\hbar^2 K^4}\left[e^{2\alpha r_0} - e^{\alpha r_0}\right] \qquad \ldots(4)$$

$$i.e.\ f(\theta) \propto \frac{1}{k^4 \sin^4 \theta/2}\,. \qquad \ldots(5)$$

It appears that in this case, $f(\theta)$ diminishes very rapidly with k and $\sin\theta/2$.

(b) For $K/\alpha \ll 1$

$$f(\theta) = \text{constant}. \qquad \ldots(6)$$

This means that scattering is isotropic under this condition.

Finally, we consider Morse scattering in presence of Coulomb field. Replacing the incident plane wave function by Coulomb wave function in the first Born approximation (Messiah, 1961), we obtain for the scattering of an ion by an ion,

$$F(\theta) = -\frac{2m}{4\pi\hbar^2}\int_0^\infty e^{-i\vec{k}'\cdot\vec{r}}\,.\,V(r),\ e^{i[\vec{k}\vec{r}+\gamma \log k(r-z)]}\,d^3\vec{r}$$

where, $\gamma = \dfrac{mZZ'e^2}{\hbar k}$; Ze, $Z'e$ being the charges of the ions. ...(7)

On calcuation (Copson 1955), it appears that due to the presence of Couloinb field, phase changes and that we obtain for the intensity of scattering,

$$|F(\theta)|^2 = \left(\frac{2mV_0}{K\hbar}\right)^2 (1+\gamma^2)\left(\frac{2\pi\gamma e^{\pi\gamma}}{e^{2\pi\gamma}-1}\right)[A^2+B^2] \qquad \ldots(8)$$

where,
$$A = e^{2\alpha r_0}(\cos\rho \sin 2\phi \cosh\gamma\phi + \sin\rho \cos 2\phi \sinh\gamma\phi)$$
$$-2e^{\alpha r_0}(\cos\sigma \sin 2\psi \cosh\gamma\psi + \sin\sigma \cos 2\psi \sinh\gamma\psi),$$
$$B = e^{2\alpha r_0}(\cos\rho \sin 2\phi \cosh\gamma\phi - \sin\rho \cos 2\phi \sinh\gamma\phi)$$
$$-2e^{\alpha r_0}(\cos\sigma \sin 2\psi \cosh\gamma\psi - \sin\sigma \cos 2\psi \sinh\gamma\psi),$$

with $\phi = \tan^{-1}(K/2\alpha)$, $\psi = \tan^{-1}(K/\alpha)$

$$\rho = \frac{\gamma}{2}\log(4\alpha^2+K^2),\ \sigma = \frac{\gamma}{2}\log(\alpha^2+K^2). \qquad \ldots(9)$$

In the absence of Coulomb field, (8) is reduced to the corresponding form given by (3). This also happens for large values of k, *i. e.* for $\ll 1$.

3. Validity of born approximation

The validity of the above calculations is conditioned (Merzbacher, 1961) by,

$$1 \gg \frac{2m}{k\hbar^2}\left|\int_0^\infty e^{ikr} \sin kr.\, V(r).\, dr\right|$$

$$= \frac{m\,|\,V_0\,|}{k\hbar^2}\left[\left\{\frac{e^{2\alpha r_0}}{2}\left(\frac{-\alpha}{\alpha^2+k^2}+\frac{1}{\alpha}\right)-2e^{\alpha r_0}\left(\frac{-\alpha}{\alpha^2+4k^2}+\frac{1}{\alpha}\right)\right\}^2\right.$$

$$\left.+\left\{\frac{e^{2\alpha r_0}}{2}\left(\frac{k}{\alpha^2+k^2}\right)-2e^{\alpha r_0}\left(\frac{2k}{\alpha^2+4k^2}\right)\right\}^2\right]^{1/2}. \quad \ldots(10)$$

For $k/\alpha \gg 1$, from (10) we have

$$1 \gg \frac{m\,|\,V_0\,|}{k\hbar^2\alpha}\left\{\frac{e^{2\alpha r_0}}{2}-2e^{\alpha r_0}\right\} \quad \ldots(11)$$

On the other hand, for $k/\alpha\ 1 \ll$ we have

$$1 \gg \frac{m\,|\,V_0\,|}{\hbar^2\alpha^2}\left\{\frac{e^{2\alpha r_0}}{2}-4e^{\alpha r_0}\right\} \quad \ldots(12)$$

The condition seems to be independent of velocity.

4. Phase shifts

In the first approximation, we now proceed to compute phase-shifts for S-and P-waves (Roman 1964). For the S-wave, we have

$$\tan\delta_0 \approx -k\int_0^\infty \{j_0\,(kr)\}^2\,V\,(r)\,r^2\,dr$$

$$= -\frac{V_0}{2k}\left[\left\{\frac{e^{2\alpha r_0}}{2\alpha}-\frac{2e^{\alpha r_0}}{\alpha}\right\}\right.$$

$$\left.-\left\{e^{2\alpha r_0}.\frac{\alpha}{2(\alpha^2+k^2)}-2e^{\alpha r_0}.\ \frac{\alpha}{\alpha^2+4k^2}\right\}\right]. \quad \ldots(13)$$

Taking k large compared to α,

$$\tan\delta_0 \approx -\frac{V_0}{4k\alpha}\left\{e^{2\alpha r_0}-4e^{\alpha r_0}\right\}$$

$$\text{i.e., } \tan\delta_0 \propto \frac{1}{k} \quad \ldots(14)$$

For the *P*-wave, we have

$$\tan \delta_1 \approx - k \int_0^\infty \{ j_1 (kr)\}^2 \, V(r) \, r^2 \, dr$$

$$= -\frac{V_0}{k}\Bigg[\frac{1}{2k^2} \Big\{ e^{2\alpha r_0}\Big(2k \tan^{-1}(k/\alpha) - \alpha \log (4\alpha^2+4k^2)$$

$$- 2\, e^{\alpha r_0}(2k \tan^{-1}(2k/\alpha) - \alpha 2 \log (\alpha^2 + 4k^2) \Big\}$$

$$-\frac{1}{k}\Big\{ e^{2\alpha r_0} \tan^{-1}(k/\alpha) - 2\, e^{\alpha r_0} \tan^{-1}(2k/\alpha) \Big\}$$

$$+\frac{1}{2}\Bigg\{\Big(\frac{e^{2\alpha r_0}}{2\alpha} - \frac{2e^{\alpha r_0}}{\alpha}\Big) + \Big(e^{2\alpha r_0} \cdot \frac{\alpha}{2(\alpha^2+k^2)}$$

$$-2\, e^{\alpha r_0} \frac{\alpha}{\alpha^2+4k^2} \Big)\Bigg\}\Bigg]. \qquad ...(15)$$

For k very large compared to α, it is found from (15) that δ_1 becomes almost equal to δ_0.

On the other hand, for low-energy scattering under the condition (Roman 1964), $l > k/\alpha$ ...(16)

we have,

$$\tan \delta_l \approx - \frac{2^{2l}\,(l!)^2}{[(2l+1)!]^2} \, k^{2l+1} \int_0^\infty V(r).\,r^{2l+2}.\,dr$$

$$= - \frac{(l!)^2}{(2l+1)} \, k^{l2+1} \, \frac{V_0}{\alpha^{2l+3}} \left[\frac{e^{2\alpha r_0}}{8} - 2^{2l+1} \, e^{\alpha r_0} \right]. \qquad ...(18)$$

Lastly, we consider Morse scattering in presence of Coulomb field as before. Replacing the spherical Bessel function by spherical Coulomb function in the first approximation (Tiezt, 1965 ; Messiah 1961), we have for the S—wave phase-shift in this case,

$$\tan \Delta_0 \approx - \frac{V_0}{k} \int_0^\infty \Big\{ \sin (kr - \gamma \log 2\, kr + \xi_0) \Big\}^2 V(r)\, dr$$

where ξ_0 = Coulomb phase-shift

$$= - \frac{V_0}{2k}\Bigg[\Big(e^{2\alpha r_0} \frac{1}{2\alpha} - 2\, e^{\alpha r_0} . \frac{1}{\alpha} \Big)$$

$$- \Bigg\{ 2 \sqrt{\frac{\pi\gamma}{2 \sinh \pi\gamma}} \cdot \Bigg[\frac{e^{2\alpha r_0 + 2\gamma\eta} \cos (A+x+\eta}{(4k^2+4\alpha^2)^{1/2}}$$

$$- 2 \,, \frac{e^{\alpha r_0 + 2\gamma\zeta} \cos (A+y+\zeta)}{(4\, k^2+\alpha^2)^{1/2}}$$

with,

$$\eta = \tan^{-1}(k/\alpha),\ \zeta = \tan^{-1}(2k/\alpha)$$
$$x = \gamma \log(4k^2 + 4\alpha^2),\ y = \gamma \log(4k^2 + \alpha^2)$$
$$A = 2\xi_o - 2\gamma \log 2k. \quad \ldots(19)$$

In the absence of Coulomb field, the formula assumes the form of (13). Also the same result is obtained for large values of k, i. e., for $\gamma \ll 1$.

5. Scattering length and cross-section

The scattering length is defined (Wu & Ohmura 1962) as

$$a = -\underset{k\to o}{Lt} \frac{\delta_o}{k} \approx V_o \underset{r\to\alpha}{Lt} \underset{k\to o}{Lt} \int_o^r \{j_o(kr)\}^2 V(r) r^2 dr$$
$$= \frac{V_o}{4\alpha^3} e^{2\alpha r_o} \left[1 - 16 e^{-\alpha r_o}\right]. \quad \ldots(20)$$

For bound states to be possible, a must be positive (Roman 1964). This means that $16e^{-\alpha r_o}$ must be < 1. For Cl_2, for example, this is satisfied. For this case, $r_o = 1{\cdot}988 \times 10^{-8}$ cm., $V_o = 2{\cdot}475$ ev, $\alpha = 4{\cdot}048/(1{\cdot}988 \times 10^{-8})$ so that $16\, e^{-\alpha r_o}$ is < 1 (Herzberg 1961). For the hydrogen molecule, however, this is not found to be satisfied (Messiah 1961). In this case, $= 0{\cdot}74 \times 10^{-8}$ cm, $V = 4{\cdot}72$ ev, $\alpha = 10^8/(0{\cdot}68 \times 0{\cdot}74)$ so that evidently $16\, e^{-\alpha r_o}$ is > 1. Because, (20) holds only for weak potentials (Roman 1964).

The zero-energy limit of the total cross-section (Roman 1964) may be obtained from (20) :

$$Lt_{k\to o}\ \sigma = 4\pi a^2 \frac{\pi V_o^2}{4\alpha^6} e^{4\alpha r_o} \left[1 - 16 e^{-\alpha r_o}\right]^2 \quad \ldots(21)$$

For very large α, this becomes

$$= \frac{\pi V_o^2}{4\alpha^6} e^{4\alpha r_o} \quad \ldots(22)$$

6. S-Wave scattering

Lastly we solve the radial wave equation for the S-wave scattering. We write the equation in the form :

$$\frac{d^2\psi}{dr^2} + (k^2 - V(r))\,\psi = 0 \qquad \dots (23)$$

Making the following substitutions

$$e^{-\alpha r} = Z$$

$$C = V_0\, e^{2\alpha r_0}/\alpha^2, \quad D = 2V_0\, e^{\alpha r_0}/\alpha^2$$

$$\psi = A e^{-ik/\alpha \log z}\, e^{-\beta z/2\alpha}\phi(z) \qquad \dots (24)$$

where β is yet undetermined, we obtain from (23)

$$z\frac{d^2\phi}{dz^2} + \left\{\left(1 - \frac{2ik}{\alpha}\right) - \frac{\beta}{\alpha} z\right\}\frac{d\phi}{dz} + \left[\frac{\beta^2}{4\alpha^2} z - \frac{\beta}{2\alpha}\left(1 - \frac{2ik}{\alpha}\right) - (Cz - D)\right]\phi = 0. \qquad \dots (25)$$

This equation may be taken in the confluent hypergeometric form (Morse & Feshbach 1953) by adjusting the value of β such that

$$\beta^2/4\alpha^2 = C. \qquad \dots (26)$$

In that case, (25) has the solution

$$\psi = A\, e^{ikr}\, e^{-\beta/2\alpha(e^{-\alpha r})}\, \phi\left[\frac{1}{2}\left(1 - \frac{2ik}{\alpha} - \frac{2\alpha D}{\beta}\right)\Big|\left(1 - \frac{2ik}{\alpha}\right)\Big|\frac{\beta}{\alpha}e^{-\alpha r}\right] \qquad \dots (27)$$

The most general solution therefore takes the form :

$$\psi = e^{-\beta/2\alpha(e^{-\alpha r})}\left\{A\, e^{ikr}\, \phi_1\left[\frac{1}{2}\left(1 - \frac{2ik}{\alpha} - \frac{2\alpha D}{\beta}\right)\Big|\left(1 - \frac{2ik}{\alpha}\right)\Big|\frac{\beta}{\alpha}e^{-\alpha r}\right]\right.$$

$$\left. + B\, e^{-ikr}\, \phi_2\left[\frac{1}{2}\left(1 + \frac{2ik}{\alpha} - \frac{2\alpha D}{\beta}\right)\Big|\left(1 + \frac{2ik}{\alpha}\right)\Big|\frac{\beta}{\alpha}e^{-\alpha r}\right]\right\} \qquad \dots (28)$$

A similar solution for the radial S-wave equation has been obtained by Bhattacharjee & Sudarsan (1962) by a different method for a potential slightly different from (2).

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